Scaling and Renormalization in Statistical Physics

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Contents

	Preface	page xiii
1	Phase transitions in simple systems	1
1.1	Phase diagrams	5
1.2	Simple models	10
	Exercises	14
2	Mean field theory	16
2.1	The mean field free energy	16
2.2	Critical exponents	20
2.3	Mean field theory for the correlation function	22
2.4	Corrections to mean field theory	24
	Exercises	26
3	The renormalization group idea	28
3.1	Block spin transformations	30
3.2	One-dimensional Ising model	34
3.3	General theory	40
3.4	Scaling behaviour of the free energy	43
3.5	Critical exponents	45
3.6	Irrelevant eigenvalues	48
3.7	Scaling for the correlation functions	49
3.8	Scaling operators and scaling dimensions	52
3.9	Critical amplitudes	55
	Exercises	59
4	Phase diagrams and fixed points	61
4.1	Ising model with vacancies	61
4.2	Cross-over behaviour	67
4.3	Cross-over to long range behaviour	71
4.4	Finite-size scaling	72
4.5	Quantum critical behaviour	76

x Contents

	Exercises	81
5 5.1	The perturbative renormalization group	83
5.2	The perturbative representation	84
5.3	The perturbative renormalization group	86
5.4	The Coursing fixed point	90
5.5	The Gaussian fixed point	92
5.6	The Wilson-Fisher fixed point	94
5.7	Logarithmic corrections in $d=4$	103
5.8	The $O(n)$ model near four dimensions Cubic symmetry breaking	104
5. 6	Exercises	107
		109
6	Low dimensional systems	111
6.1	The lower critical dimension	111
6.2	The two-dimensional XY model	113
6.3	The solid-on-solid model	117
6.4	Renormalization group analysis	120
6.5	The $O(n)$ model in $2+\epsilon$ dimensions	127
	Exercises	131
7	Surface critical behaviour	133
7.1	Mean field theory	134
7.2	The extraordinary and special transitions	136
7.3	Renormalization group approach	138
	Exercises	144
8	Random systems	
8.1	Quenched and annealed disorder	145
8.2	The Harris criterion	145
8.3	Perturbative approach to the random fixed point	148
8.4	Percolation	$150 \\ 153$
8.5	Random fields	161
0.0	Exercises	167
9	Polymer statistics	
9.1	Random walk model	169
$9.1 \\ 9.2$	The Edwards model and the Flory formula	169
9.2	Mapping to the $O(n)$ model	170
9.4	Finite concentration	172
9.5	Other applications	177

Contents	Xì
Exercises	181
Critical dynamics	183
Continuum models	186
Discrete models	189
Dynamic scaling	192
Response functional formalism	193
Other dynamic universality classes	196
Directed percolation	200
Exercises	204
Conformal symmetry	206
Conformal transformations	209
Simple consequences of conformal symmetry	211
The stress tensor	215
Further developments	222
The c-theorem	223
Exercises	225
Appendix: Gaussian integration	227
Selected bibliography	229
Index	234
	Critical dynamics Continuum models Discrete models Dynamic scaling Response functional formalism Other dynamic universality classes Directed percolation Exercises Conformal symmetry Conformal transformations Simple consequences of conformal symmetry The stress tensor Further developments The c-theorem Exercises Appendix: Gaussian integration Selected bibliography

Phase transitions in simple systems

Take a large piece of material and measure some of its macroscopic properties, for example its density, compressibility or magnetisation. Now divide it into two roughly equal halves, keeping the external variables like pressure and temperature the same. The macroscopic properties of each piece will then be the same as those of the whole. The same holds true if the process is repeated. But eventually, after many iterations, something different must happen, because we know that matter is made up of atoms and molecules whose individual properties are quite different from those of the matter which they constitute. The length scale at which the overall properties of the pieces begin to differ markedly from those of the original gives a measure of what is termed the correlation length of the material. It is the distance over which the fluctuations of the microscopic degrees of freedom (the positions of the atoms and suchlike) are significantly correlated with each other. The fluctuations in two parts of the material much further apart than the correlation length are effectively disconnected from each other. Therefore it makes no appreciable difference to the macroscopic properties if the connection is completely severed.

Usually the correlation length is of the order of a few interatomic spacings. This means that we may consider really quite small collections of atoms to get a very good idea of the macroscopic behaviour of the material. (This statement needs qualification. In reality, small clusters of atoms will exhibit very strong surface effects which may be quite different from, and dominate, the bulk behaviour. However, since this is only a thought experiment, we may imagine employing the theoretician's device of periodic boundary conditions, thereby eliminating them.) However, the actual value of the correlation length depends on the external conditions determining the state of the system, such as the temp-

erature and pressure. It is well known that systems may abruptly change their macroscopic behaviour as these quantities are smoothly varied. The points at which this happens are called critical points, and they usually mark a phase transition from one state of matter to another. There are basically two possible ways in which such a transition may occur. In the first scenario, the two (or more) states on either side of the critical point also coexist exactly at the critical point. However, even then they are distinct from each other, in that they have different macroscopic properties. Slightly away from the critical point, however, there is generically a unique phase whose properties are continuously connected to one of the co-existent phases at the critical point. In that case, we should expect to find discontinuous behaviour in various thermodynamic quantities as we pass through the critical point, and therefore from one stable phase to another. Such transitions are termed discontinuous or first-order. Well-known examples are the melting of a three-dimensional solid, or the condensation of a gas into a liquid. In fact, such transitions often exhibit hysteresis. or memory effects, since the continuation of a given state into the opposite phase may be metastable so that the system may take a macroscopically long time to readjust. The correlation length at such a first-order transition is generally finite.

However, the situation is quite different at a continuous transition, where the correlation length becomes effectively infinite. The fluctuations are then correlated over all distance scales, which thereby forces the whole system to be in a unique, critical, phase. At a continuous transition, therefore, the two (or more) phases on either side of the critical point must become identical as it is approached. Not only does the correlation length diverge in a continuous fashion as such a critical point is approached, but the differences in the various thermodynamic quantities between the competing phases, like the energy density and the magnetisation, go to zero smoothly. It is the task of the theory to explain this behaviour in a quantitative manner. Simple examples of continuous transitions, to be described in more detail below, occur at the Curie temperature in a ferromagnet, and at the liquid—gas critical point in a fluid.

The fact that a very large number of degrees of freedom are strongly correlated with each other makes the study of continu-

ous phase transitions intrinsically difficult. By their nature, these phenomena are not amenable to normal perturbative methods. It is only within the last twenty-five years or so that analytic methods have been developed for dealing with such problems. These methods constitute a whole new way of thinking about such phenomena, which is called the *renormalization group*.

Although systems with large correlation lengths might appear to be very complex, they also exhibit some beautiful simplifications. One of these is the phenomenon of universality. Many properties of a system close to a continuous phase transition turn out to be largely independent of the microscopic details of the interactions between the individual atoms and molecules. Instead, they fall into one of a relatively small number of different classes, each characterised only by global features such as the symmetries of the underlying hamiltonian, the number of spatial dimensions of the system, and so on. This phenomenon finds a simple and natural explanation within the framework of the renormalization group. Typically, close to a critical point, the correlation length and the other thermodynamic quantities exhibit power-law dependences on the parameters specifying the distance away from the critical point. These powers, or critical exponents, are pure numbers, usually not integers or even simple rational numbers, which depend only on the universality class. One of the basic theoretical challenges, then, is to explain why such non-trivial powers should occur, and to predict their actual values.

The occurrence of power behaviour in the laws describing a system is a symptom of scaling behaviour. Such dependences occur, of course, in problems at many levels in the physical sciences. In the most elementary cases, they are simply the result of dimensional analysis. For example, once the inverse square law $1/r^2$ for the gravitational acceleration of a body a distance r from a point mass is assumed, Kepler's law that the orbital period $T \propto r^{3/2}$, follows immediately. (Note that, in general, such elementary arguments lead to simple rational numbers for the exponents.) However, most physical problems present us with more than one length scale, and simple dimensional analysis is no longer adequate. Physical quantities may then depend in an arbitrarily complicated manner on the dimensionless ratios of these scales. Nevertheless, simplifications may occur if there is a wide $separation \ of \ scales$ in the

problem. In that case, it may be permissible to neglect the shorter length scales when discussing the large scale physics. This, in fact, already occurs in the problem of planetary motion, where it may be shown that the finite radius of the bodies has no significant effect.

Similar results follow in the so-called 'classical' approaches to the problem of continuous phase transitions. The approximate theory to be developed in Chapter 2 implies that, close to the critical point of a ferromagnet, the correlation function G(r) of the local fluctuations in the magnetisation obeys Laplace's equation over distance scales r much less than the correlation length ξ , and therefore exhibits a 1/r behaviour in three dimensions, like the gravitational potential. This problem would appear to have two potentially important length scales: the microscopic length a which specifies the typical distance between the fluctuating magnetic degrees of freedom, and the correlation length ξ . Thus, we might be tempted to argue, in analogy with the planetary problem, that when $\xi \gg a$, that is, very close to the critical point, the microscopic length a may be ignored. Under that assumption, dimensional analysis then implies that a has the form

$$G(r) = \frac{1}{r}f(r/\xi),\tag{1.1}$$

where f is some function, as yet unknown. From the magnetic correlation function, we may infer the susceptibility $\chi \propto \int G(r)d^3r$. Substituting in the above form, we then find, after a change of integration variables, that $\chi \propto \xi^2$. This simple power law is essentially a consequence of dimensional analysis, and is a typical result of the 'classical' approach to critical behaviour, which predates the renormalization group.

However, both experiments and studies of simplified lattice models indicate that the above result is incorrect. The reason is that, unlike the Kepler problem, critical behaviour is dominated by the effects of fluctuations, and these fluctuations take place on all length scales, all the way down to the microscopic distance a. It is therefore not permissible simply to neglect a, even when it is much smaller than the characteristic length ξ . It might then appear that little more can be said without further detailed analysis.

since (1.1) is now replaced by the weaker relation

$$G(r) = \frac{1}{r} f(r/\xi, a/\xi).$$
 (1.2)

However, it turns out that, for $a/\xi \ll 1$, although the function f is not independent of this ratio, it nevertheless exhibits a simple power law dependence, proportional to $(a/\xi)^{\eta}$, where η is a small but non-zero exponent. As a consequence, the dependence of the susceptibility on the correlation length has the form

$$\chi \propto a^{\eta} \, \xi^{2-\eta}. \tag{1.3}$$

Thus, scaling is, in a sense, recovered, but with an exponent $2-\eta$ which does not follow from straightforward dimensional analysis. The deviation η is an example of an anomalous dimension. The existence of such behaviour demands, of course, an explanation. It will turn out that this arises quite naturally within the framework of the renormalization group.

Before discussing these general properties further, however, it is useful to have at hand some very simple physical examples of continuous critical behaviour in which these concepts may be illustrated in a concrete fashion.

1.1 Phase diagrams

Uniaxial ferromagnets

In a ferromagnet there are two interesting external parameters which may be varied: the temperature T and the applied magnetic field H. In the most straightforward case, the local magnetisation is constrained to lie parallel or anti-parallel to a particular axis. The phase diagram (Figure 1.1) is simple. All the thermodynamic quantities (e.g. specific heat, susceptibility) are smooth analytic functions of T and H except on the line $H=0, T \leq T_c$. Across the line $T < T_c$, the magnetisation M, as a function of H, is discontinuous, having the form illustrated in Figure 1.2a. This discontinuity is characteristic of a first-order transition, with a finite correlation length. As T approaches the Curie point T_c , from below, however, the discontinuity approaches zero, and the correlation length at the transition diverges. The point $H=0, T=T_c$ is an example of a critical end point, at which the first-order transition becomes continuous.

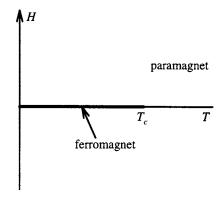


Figure 1.1. Phase diagram of a uniaxial ferromagnet.

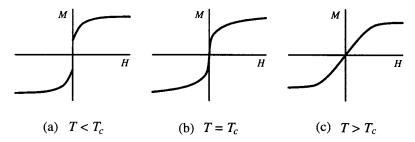


Figure 1.2. Magnetisation versus applied field, for various temperatures.

When $T < T_c$, the two limits $H \to 0+$ and $H \to 0-$ give different possible values $\pm M_0$ for the magnetisation. Which one the system chooses depends on its previous history. This is an example of spontaneous symmetry breaking: although the hamiltonian is invariant under simultaneous reversal of all the local magnetic degrees of freedom, this symmetry is not respected by the equilibrium thermodynamic state. The onset of such symmetry breaking is a common, although not a universal, characteristic of continuous critical points. The magnetisation M, whose value measures the amount of magnetic order in the material, is called the order parameter for this transition. In most, but not all, examples of critical behaviour, it is possible to identify one or more such order parameters, and the behaviour of their local fluctuations often provides a useful way of characterising the nature of the transition.

As mentioned above, most of the quantities of interest exhibit power law behaviour sufficiently close to the critical point. We now give the definitions of the principal critical exponents which characterise these power laws for the case of a ferromagnet. It is useful to define two dimensionless measures of the deviation from the critical point: the reduced temperature $t \equiv (T - T_c)/T_c$, and the reduced external magnetic field $h = H/k_BT_c$. The exponents are

- α : The specific heat in zero field $C \sim A|t|^{-\alpha}$, apart from terms which are regular in t. Note that, in principle, one should consider the possibility of different exponents α and α' for t>0 and t<0 respectively. However, it is an immediate consequence of the renormalization group (in agreement with other exact results) that $\alpha=\alpha'$, and we shall henceforth cease to make a distinction. α can be positive or negative, corresponding to either a divergent spike or a cusp in the specific heat when plotted against T. Although the exponent α is universal, the amplitude A is not, and, moreover, $A \neq A'$ in general. However, a prediction of the renormalization group is that the ratio A'/A is universal (see Section 3.9).
- β : The spontaneous magnetisation $\lim_{H\to 0+} M \propto (-t)^{\beta}$.
- γ : Zero field susceptibility $\chi \equiv (\partial M/\partial H)|_{H=0} \propto |t|^{-\gamma}$. Once again, in principle different exponents should be defined for different signs of t, but in fact theory indicates that they should be equal.
- δ : At $T = T_c$, the magnetisation varies with h according to $M \propto |h|^{1/\delta}$.
- ν : A more quantitative measure of the correlation length ξ than given above is through the asymptotic behaviour $G(r) \propto e^{-r/\xi}/r^{(d-1)/2}$ (for $r \gg \xi$) of the correlation function of the fluctuations in the local magnetisation. Alternatively, it may be defined through the second moment of this quantity, $\xi^2 = \sum_r r^2 G(r)/\sum_r G(r)$. In either case, it diverges as $t \to 0$, with h=0, according to $\xi \propto |t|^{-\nu}$. Once again, this has a meaning either side of the critical point.
- η : Exactly at the critical point, the correlation function does not decay exponentially, but rather according to $G(r) \propto 1/r^{d-2+\eta}$.

z: Finally, there is an exponent relating to the time-dependent properties close to the critical point. For example, the typical relaxation time τ diverges, as the critical point is approached, according to $\tau \propto \xi^z$. Since this exponent does not relate to the static equilibrium properties, however, further discussion will be deferred until Chapter 10.

This completes the commonly observed zoo of exponents for this critical point. Although this nomenclature has come to be accepted for historical reasons, it will become clear in Chapter 3 that these critical exponents are not the most fundamental quantities from the theoretical perspective. Rather, they are simply derived from a smaller set of numbers called the scaling dimensions.

Many of the definitions given above may be taken over without modification to the Curie point in more general ferromagnets, for example Heisenberg magnets where the local moments are free to rotate in three dimensions. The only difference is in the low-temperature phase, when a distinction must be drawn between fluctuations of the local magnetisation parallel to, and perpendicular to, the direction of the spontaneous magnetisation. In this case, the transverse susceptibility, the response of the magnetisation to an applied field perpendicular to the spontaneous magnetisation, remains infinite throughout the low-temperature phase, and the critical exponent γ must then be defined in terms of the longitudinal susceptibility only. Similar generalisations apply to the vicinity of the Néel point in antiferromagnets. In this case, it is the sublattice, or staggered, magnetisation which plays the role of the order parameter.

Simple fluids

The phase diagram of a generic substance in the temperaturepressure plane usually has the form shown in Figure 1.3. Let us focus on the part of the phase diagram close to the liquid–gas critical point at (T_c, p_c) . It looks quite similar to that for the ferromagnet in the (T, H)-plane. Across the liquid–gas phase boundary, the density ρ is discontinuous. The jump in the density $\rho_{\text{liquid}}-\rho_{\text{gas}}$ approaches zero at the critical end point (T_c, p_c) . The isotherms, curves of p versus ρ at constant T, are illustrated in Figure 1.4.

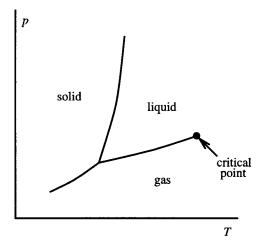


Figure 1.3. Phase diagram of a typical substance.

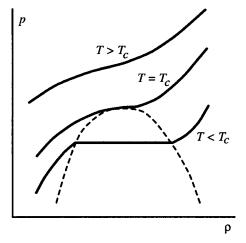


Figure 1.4. Isotherms near the liquid-gas critical point. The dashed line is the coexistence curve.

Comparing this with the graphs of the magnetisation in a ferromagnet shown in Figure 1.2, we see that $p-p_c$ is analogous to the applied field H, and $\rho-\rho_c$ to the magnetisation M. The main physical difference between the systems is that, in a fluid the overall average density is usually fixed. This means that, underneath the coexistence curve shown in Figure 1.4, the system separates

into two coexisting phases, the relative volume occupied by each being determined by their densities and the total mass. For a magnet, however, the total magnetisation is not usually fixed by the conditions of the experiment.

The critical exponents at the liquid-gas critical point are therefore defined in analogy to those for the magnet:

- $C_V \propto |t|^{-\alpha}$ at $\rho = \rho_c$;
- $\rho_L \rho_G \propto (-t)^{\beta}$ gives the shape of the coexistence curve near the critical point;
- isothermal compressibility $\chi_T \propto |t|^{-\gamma}$;
- $p-p_c \propto |\rho_L-\rho_G|^{\delta}$ gives the shape of the critical isotherm near the critical point.

The exponents ν and η are defined as for the ferromagnet, with G(r) now being the density-density correlation function.

One of the most remarkable results of universality is that the critical exponents of a simple fluid are identical with those of uniaxial ferromagnets.

1.2 Simple models

These equilibrium systems with many degrees of freedom, are, of course, governed by the laws of statistical mechanics. This means that the mathematical problem is at least well-defined. Physical quantities are given in terms of averages with respect to the Gibbs distribution $e^{-\beta \mathcal{H}}$.† In particular, thermodynamic quantities such as the specific heat or the magnetisation are given by suitable derivatives of the partition function

$$Z = \text{Tr}e^{-\beta \mathcal{H}},\tag{1.4}$$

or, equivalently, of the free energy $F = -\beta^{-1} \ln Z$. Even when the hamiltonian \mathcal{H} is relatively simple, computing Z is usually very difficult. For a realistic hamiltonian, it is a hopeless task. This has led to the consideration of drastically simplified models which, it is hoped, nonetheless capture the essential physics. However, there is a unique advantage in approaching these kinds of problem through the study of models, which is not present in most areas of physics.

[†] There should be no confusion between $\beta \equiv (k_B T)^{-1}$ and the critical exponent denoted by the same symbol.

In the study of atomic phenomena, for example, one tries to invent a model which is as close to the true hamiltonian as possible, but is nevertheless solvable, exactly or approximately. Once the parameters have been suitably adjusted, the results of such studies are then expected to match the observed phenomena closely, but, not of course exactly, since any model inevitably omits some effects. Once rough agreement has been obtained, the model may then be refined, so as to improve the accuracy of the description.

However, because of the phenomenon of universality in critical phenomena, one may hope to obtain results from very simple models which exactly match the behaviour of real systems, at least in those aspects which are universal. Moreover, in general, these universal features should be independent of the microscopic parameters of the model, and there is therefore no question of parameter-fitting: the theory is either right or wrong. In reality the situation is not quite as simple as this. Real or numerical experiments never probe the true asymptotic region close to the critical point, and therefore so-called corrections to scaling, which contain non-universal and therefore adjustable parameters, often need to be incorporated to obtain a good fit. Nevertheless, it is true that theoretical models of critical behaviour may be tested with much greater precision than occurs in most other areas of condensed matter physics.

Even so, only a few of the simplest models in low dimensions may be solved exactly, and although the mathematical methods involved constitute a fascinating subject in their own right, the details of this analysis have little bearing on the kinds of question the physicist would like to have answered. This is partly because the exact solution of a model does not, in general, differentiate between those results which are universal and those which are not. It is then by no means clear which properties of the exact solution of the simplified model are supposed to carry over to real systems. However, the renormalization group approach does make such a distinction, through the arguments we shall develop in Chapter 3. From this point of view, then, model hamiltonians are more usefully regarded as frameworks within which to describe the important microscopic features of a given universality class, rather than as objects for exact solution.

An immediate simplification which may be made in almost all

systems comes from the observation that, at finite temperatures, the critical thermal fluctuations completely dominate the quantum mechanical ones. This statement will be made more quantitative in Section 4.5. Thus, the simplified models we study are almost always described by a *classical* hamiltonian \mathcal{H} , and the calculation of the partition function involves a sum over classical phase space. This is true even though the underlying physics driving the phenomena (e.g. magnetic exchange interactions, superfluidity) may be intrinsically quantum mechanical in nature.

Magnets

The simplest way of modelling a ferromagnet is to imagine quantum mechanical spins $\mathbf{s}(r)$ localised on the sites r of a lattice. The spins interact in pairs with a hamiltonian $\mathcal{H} = -\frac{1}{2} \sum_{r,r'} J(r,r')$ $\mathbf{s}(r) \cdot \mathbf{s}(r')$, where J(r,r') falls off with the distance between r and r'. If J>0 the interaction is ferromagnetic. Application of an external magnetic field corresponds to the addition of a term $-\mu \mathbf{H} \cdot \sum_r \mathbf{s}(r)$. This model is the quantum Heisenberg model. For the reasons mentioned above, however, at finite temperature we may ignore the quantum aspect of the spins, and regard the $\mathbf{s}(r)$ as classical objects whose configuration space corresponds to the points on the surface of a sphere.

In a real system the spins usually lie in a crystalline lattice which does not possess full rotational symmetry. There may then be crystalline fields acting on the spins which make them prefer to align along certain axes. In the case of uniaxial anisotropy, the spins prefer to lie along, for example, the z-axis, and we may then restrict the allowed values of the degrees of freedom to be $s^z(r) = \pm 1$, in suitable units. This gives the Ising model, perhaps the most famous and fundamental model of critical behaviour. Alternatively, the spins may prefer to lie down in the xy-plane, so that s(r) has only two components, satisfying $s^x(r)^2 + s^y(r)^2 = 1$. This gives the XY or planar model.

The XY model has another important realisation. In superfluid helium, a finite fraction of the degrees of freedom of the system condense into a macroscopic quantum state, whose wave function $\Psi(r)$ is a complex number. It turns out that for most purposes we may ignore its quantum mechanical origin and treat Ψ as a

classical field. Moreover, it is the fluctuations in the phase of Ψ , rather than in its modulus, which dominate the transition into the normal state. Thus we may regard the length of Ψ as fixed. Moreover, the short-range repulsion between the helium atoms may be modelled by localising the degrees of freedom to lie on a lattice, thereby arriving at a model mathematically identical to the XY model. Similar considerations apply to superconductors, which also provide examples of the XY universality class.

More generally, we may consider a spin having n components. This gives the n-vector or O(n) model. The above three cases correspond to n=3,1,2 respectively, but it is mathematically possible to think about this model for arbitrary n. As we shall see in Chapter 9, even the limit $n\to 0$ has a physical interpretation in describing the statistics of long polymer chains.

Fluids

A simple classical fluid may be specified by the positions r_1, \ldots, r_N of its N particles. It is often convenient to work in the grand canonical ensemble, in which case the grand partition function is

$$\Xi = \sum_{N} \frac{\zeta^{N}}{N!} \int e^{-\beta \sum_{i < j} V(r_{i} - r_{j})} d^{3}r_{1} \dots d^{3}r_{N}, \qquad (1.5)$$

where ζ is proportional to the fugacity, and we consider only a two-body interaction V, which is supposed to be short-ranged and attractive, with a hard core repulsive component. This model is already quite difficult to analyse using renormalization group methods, and it is common to replace it with an idealisation called the lattice gas model. The particles are now assumed to occupy the sites r of a regular lattice, and the hard core interaction is modelled by restricting the occupation number n(r) to take only the values 0 or 1. The attractive part of the potential is described by the interaction $-2\sum_{r,r'}J(r,r')n(r)n(r')$, where J>0. Then

$$\Xi = \sum_{n(r)=0,1} \zeta^{\sum_{r} n(r)} e^{2\beta \sum_{r,r'} J(r,r')n(r)n(r')}.$$
 (1.6)

This may be cast in a more familiar form by defining s(r) = 2n(r) - 1, which takes the values ± 1 . The terms in the exponential

in (1.6) are then, apart from an unimportant constant,

$$\frac{1}{2}\beta \sum_{r,r'} J(r,r')s(r)s(r') + \beta H \sum_{r} s(r), \qquad (1.7)$$

where $H = \frac{1}{2}k_BT\ln\zeta + \sum_{r'}J(r,r')$. This is the hamiltonian for the Ising model in a magnetic field! Thus, as long as the various rather crude approximations which led to this result are justified on the grounds of universality, the simple liquid-gas critical point and the Curie point of uniaxial ferromagnets should be in the same universality class, described by the simple Ising model. It is interesting to note that the hamiltonian of the Ising model in zero field has a symmetry under simultaneous reversal of all the spins $s(r) \rightarrow -s(r)$. It is this symmetry which is broken spontaneously below the critical temperature. However, the simple fluid has, in general, no such symmetry in its microscopic dynamics. It is only close to the critical point that this symmetry emerges. For example, the isotherms in Figure 1.4 are symmetrical under reflection about the point (ρ_c, p_c) only close to this point. This is an example of a common property of critical systems, that their symmetries are often enhanced in the critical region. This has a natural explanation within the framework of the renormalization group.

There are several other common systems in the Ising universality class. For example, a binary fluid, consisting of two components which are miscible above a certain critical temperature, and phase separate below it, has a phase diagram very similar to that of Figure 1.4, with ρ now representing the relative density of one of the components. Similarly, many structural phase transitions in crystals are Ising-like. However, we should issue the warning that such identifications are usually limited to the *static* equilibrium behaviour. As we shall see in Chapter 10, the critical dynamics of these systems may be quite different from each other.

Exercises

1.1 In a model of a binary alloy, each site of the lattice may be occupied by a particle of type A or one of type B. The interactions between the different types of particle are given by $J_{AA}(r-r')$, $J_{BB}(r-r')$ and $J_{AB}(r-r')$. Map this problem

Exercises 15

to an Ising model by assigning a variable s(r) to each site, which takes the values +1 or -1 according to the two cases described above. For what ranges of the interaction parameters should we expect to see critical behaviour of the Ising type?

- 1.2 An Ising antiferromagnet may be described by the hamiltonian discussed in the text on p.12, with J(r,r') < 0. Show that, on a hypercubic lattice, when the dominant interactions are between nearest neighbours, it is possible by a redefinition of variables to map this problem into that of a ferromagnet, so that they are therefore in the same universality class. What happens, for example, on a triangular lattice?
- 1.3 Real antiferromagnets have magnetic ions with quantum mechanical spins of spin S, not necessarily equal to $\frac{1}{2}$, and exchange interaction J. How would you map (approximately) such a model onto the usual spin- $\frac{1}{2}$ Ising model with some effective exchange interaction J_{eff} ? [Hint: compare their behaviours at high temperature.]
- 1.4 Atoms of a rare gas are adsorbed on a substrate. The adsorbed atoms occupy the sites of a square lattice: however, the radius of the adsorbed atoms is such that neighbouring sites of the square lattice cannot be simultaneously occupied. Show that at high densities and low temperature there are two possible degenerate ground states for this system, and hence deduce the form of the phase diagram in analogy with that of the Ising model. How would the phase transition show up in the structure factor as measured, say, by X-ray or low energy electron diffraction?